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Bound States of the Relativistic Rotating Deng-Fan Oscillator Potential

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Abstract

The generalized Morse or Deng-Fan Potential describes diatomic molecular energy spectra and electromagnetic transitions. We solve the Klein-Gordon (K-G) equation for Deng-Fan Potential in arbitrary N -dimension and use an improved approximation scheme to the centrifugal term. By using the generalized parametric Nikiforov-Uvarov (NU) method, we obtain the energy eigenvalues and corresponding wave functions in closed forms. The effect of potential parameters and the dimension N on the energy eigenvalues is numerically discussed.

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1. Introduction

In the twenty last years, great attentions paid to solve K-G and Dirac equations for various quantum systems. Also, the exact analytic solutions of the wave functions are only possible for certain potentials such as Coulomb, harmonic, Mie-type and pseudoharmonic potentials [1-5]. The analytic exact solutions of the wave functions with some exponential-type are possible for $l = 0$ cases and approximation solutions have to be used to the centrifugal terms such as Pekeris approximation [6] and the approximation scheme suggested by Greene and Aldrich [7]. Many authors used

different methods to study the exactly and approximately solvable Schrödinger, K-G and Dirac equations in one-, 3- and/or any N -dimensional cases for different potentials [8-25].
The Deng-Fan potential suggested by Deng and Fan is rotating potential defined by [26]

$$V(r) = D\left(1-\frac{b}{e^{ar}-1}\right)^2, \quad b = e^{ar_e}-1, \tag{1}$$

where $r \in (0,\infty)$ and D , r_e and a denote the dissociation energy, equilibrium inter-nuclear distance and range of the potential well, respectively. The Deng-Fan Potential describes diatomic molecular energy spectra and electromagnetic transitions [27].
Dong and Gu approximately presented the bound state solutions of the Schrödinger equation with the rotating Deng-Fan molecular potential [28]. Mesa et al. studied the bound state spectrum of Deng-Fan potential by an $so(2,2)$ symmetry algebra and calculated the Frank-Gondon factors for electromagnetic transition between rovibrational levels based on different electronic states [27]. Very recently, Ikhdair solved the Dirac equation for the generalized Morse potential with arbitrary spin-orbit quantum number κ [29].
In this paper, we investigate K-G equation for Deng-Fan potential in arbitrary N -dimension, by using an improved approximation scheme to deal with the centrifugal term. We use the generalized parametric NU method to obtain energy eigenvalues and corresponding eigenfunctions. Thus, this paper is arranged as follows: in section 2, we give a brief introduction to K-G equation in N -dimension. In section 3, The NU method is briefly introduced. The generalized parametric NU method is displayed in appendix A. In section 4, we solve hyperradial K-G equation with Deng-Fan potential by the mentioned method. Some numerical results are given in this section, too. Finally, our conclusions are given in section 5.

2. K-G equation in N -dimension

In spherical coordinates, the K-G equation with vector potential $V(r)$, and scalar one $S(r)$, is written as $[\hbar = c = 1]$

$$-\Delta_N \psi_{nlm}(r,\Omega_N) = \left[\left(E_{nl} - V(r)\right)^2 - \left(m - S(r)\right)^2\right]\psi_{nlm}(r,\Omega_N), \tag{2}$$

with

$$\Delta_N = \nabla_N^2 = \frac{1}{r^{N-1}}\frac{\partial}{\partial r}\left(r^{N-1}\frac{\partial}{\partial r}\right) - \frac{\Lambda_N^2(\Omega_N)}{r^2}, \tag{3}$$

where E_{nl}, $\frac{\Lambda_N^2(\Omega_N)}{r^2}$ and Ω_N are the energy eigenvalues, a generation of the centrifugal barrier for N -dimension and the angular coordinates, respectively. The eigenvalues of the $\Lambda_N^2(\Omega_N)$ are given by

$$\Lambda_N^2(\Omega_N) Y_l^m(\Omega_N) = l(l+D-2) Y_l^m(\Omega_N), \tag{4}$$

where $Y_l^m(\Omega_N)$ is the hyperspherical harmonics. Using separation variables method with the wave function $\psi_{nlm}(r,\Omega_N)=\frac{R_{nl}(r)}{r}Y_l^m(\Omega_N)$, Eq. (2) reduces to

$$\left[\frac{d^2}{dr^2}+E_{n,l}{}^2+V^2(r)-2E_{n,l}V(r)-m^2(r)-S^2(r)-2m(r)S(r)\right.$$
$$\left.-\frac{(N+2l-1)(N+2l-3)}{4r^2}\right]R_{n,l}(r)=0. \tag{5}$$

When vector potential $V(r)$ is equal to the scalar potential $S(r)$, lead us to obtain a Schrödinger-like equation as

$$\left[\frac{d^2}{dr^2}+\varepsilon^2-2(E_{nl}-m)V(r)-\frac{(N+2l-1)(N+2l-3)}{4r^2}\right]R_{n,l}(r)=0, \tag{6}$$

where $\varepsilon^2=E_{nl}^2-m^2$. Because of the centrifugal term in above equation, we can not solve it exactly. By using the following improved new approximation scheme to the centrifugal term near the minimum point $r=r_e$, as [29]

$$\frac{1}{r^2}\approx a^2\left(d_0+\frac{1}{e^{ar}-1}+\frac{1}{(e^{ar}-1)^2}\right), \tag{7}$$

where $d_0=\frac{1}{12}$, Eq. (6) can be solvable and with substitution of Eq. (1), it becomes as follows

$$\left[\frac{d^2}{dr^2}+\varepsilon^2-2(E_{nl}-m)D\left(1-\frac{b}{e^{ar}-1}\right)^2\right.$$
$$\left.-\frac{a^2(N+2l-1)(N+2l-3)}{4}\left(d_0+\frac{1}{e^{ar}-1}+\frac{1}{(e^{ar}-1)^2}\right)\right]R_{n,l}(r)=0. \tag{8}$$

To solve Eq. (8), we use the and its generalized parametric NU method.

3. Generalized Parametric Nikiforov-Uvarov method

To solve second order differential equations, the Nikiforov-Uvarov method can be used with an appropriate coordinate transformation $s=s(r)$ [30]

$$\psi_n''(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s)=0, \tag{9}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most of second-degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. The following equation is a general form of the Schrödinger-like equation written for any potential [31]

$$\left[\frac{d^2}{ds^2}+\frac{\alpha_1-\alpha_2 s}{s\left(1-\alpha_3 s\right)}\frac{d}{ds}+\frac{-\xi_1 s^2+\xi_2 s-\xi_3}{\left[s\left(1-\alpha_3 s\right)\right]^2}\right]\psi_n\left(s\right)=0. \tag{10}$$

According to the Nikiforov-Uvarov method, the eigenfunctions and eigenenergy function become, respectively

$$\psi\left(s\right)=s^{\alpha_{12}}\left(1-\alpha_3 s\right)^{-\alpha_{12}-\frac{\alpha_{13}}{\alpha_3}}P_n^{(\alpha_{10}-1,\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}\left(1-2\alpha_3 s\right), \tag{11}$$

$$\begin{aligned}\alpha_2 n-\left(2n+1\right)\alpha_5+\left(2n+1\right)\left(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8}\right)+n\left(n+1\right)\alpha_3 \\ +\alpha_7+2\alpha_3\alpha_8+2\sqrt{\alpha_8\alpha_9}=0,\end{aligned} \tag{12}$$

where

$$\begin{aligned}&\alpha_4=\frac{1}{2}\left(1-\alpha_1\right), && \alpha_5=\frac{1}{2}\left(\alpha_2-2\alpha_3\right),\\ &\alpha_6=\alpha_5^2+\xi_1, && \alpha_7=2\alpha_4\alpha_5-\xi_2,\\ &\alpha_8=\alpha_4^2+\xi_3, && \alpha_9=\alpha_3\alpha_7+\alpha_3^2\alpha_8+\alpha_6,\end{aligned} \tag{13}$$

and

$$\begin{aligned}&\alpha_{10}=\alpha_1+2\alpha_4+2\sqrt{\alpha_8}, && \alpha_{11}=\alpha_2-2\alpha_5+2\left(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8}\right),\\ &\alpha_{12}=\alpha_4+\sqrt{\alpha_8}, && \alpha_{13}=\alpha_5-\left(\sqrt{\alpha_9}+\alpha_3\sqrt{\alpha_8}\right).\end{aligned} \tag{14}$$

In some problems $\alpha_3=0$. For this type of problems when

$$\lim_{\alpha_3\to 0}P_n^{(\alpha_{10}-1,\frac{\alpha_{11}}{\alpha_3}-\alpha_{10}-1)}\left(1-\alpha_3\right)s=L_n^{\alpha_{10}-1}\left(\alpha_{11}s\right), \tag{15}$$

and

$$\lim_{\alpha_3\to 0}\left(1-\alpha_3 s\right)^{-\alpha_{12}-\frac{\alpha_{13}}{\alpha_3}}=e^{\alpha_{13}s}, \tag{16}$$

the solution given in Eq. (9) becomes as [31]

$$\psi\left(s\right)=s^{\alpha_{12}}e^{\alpha_{13}s}L_n^{\alpha_{10}-1}\left(\alpha_{11}s\right). \tag{17}$$

4. Solution of hyperradial K-G equation with Deng-Fan potential

To solve Eq. (8), by using an appropriate transformation as $s=\frac{1}{e^{ar}-1}$, we rewrite it as follows

$$\frac{d^2R_{nl}(r)}{dr^2}+\frac{1+2s}{s(1+s)}\frac{dR_{nl}(r)}{dr}+\frac{1}{s^2(1+s)^2}\left[-\xi_1 s^2+\xi_2 s-\xi_3\right]R_{nl}(r)=0, \tag{18}$$

where

$$\xi_1 = \frac{1}{a^2}\left[2(E+m)Db^2 + \frac{a^2(N+2l-1)(N+2l-3)}{4}\right],$$
$$\xi_2 = \frac{1}{a^2}\left[2(E+m)Db + \frac{a^2(N+2l-1)(N+2l-3)}{4}\right], \tag{19}$$
$$\xi_3 = \frac{1}{a^2}\left[2(E+m)D + \frac{a^2(N+2l-1)(N+2l-3)}{4}d_0 - \varepsilon^2\right].$$

Comparing Eq. (14) and Eq. (A1), we can easily obtain the coefficients α_i ($i=1,2,3$) as follows

$$\alpha_1 = 1,\ \alpha_2 = 2,\ \alpha_3 = -1. \tag{20}$$

The values of coefficients α_i ($i = 4,5,...,13$) are found from Eqs. (13-14) and displayed in table 1. By using Eq. (12), we can obtain the closed form energy eigenvalues of the Deng-Fan potential as

$$\begin{aligned} &2(n+1)(\sqrt{\xi_1+\xi_2+\xi_3+4} - \sqrt{\xi_3}) \\ &\qquad + 2\sqrt{\xi_3(\xi_1+\xi_2+\xi_3+4)} - \xi_2 - 2\xi_3 - (n^2+3n+2) = 0. \end{aligned} \tag{21}$$

Some numerical results are given in table 2 and figures 1-3. The potential parameters are taken from Ref. [28] and $m = 1fm^{-1}$. In table 2, we calculated bound state energy with $r_e = 0.4fm$ for various a and N. In fig 1, we plotted energy eigenvalues as a function of range of the potential well a, $N = 3$ and $r_e = 0.4fm$. We see that when a increase, the energy increase too and when n and/or l increase the a affect more (green line). In fig 2, the effect of equilibrium inter-nuclear distance r_e, $N = 3$ and $a = 0.05fm^{-1}$ is shown. When r_e increase the energy decrease and it has more effect on states with higher n and/or l (for example; compare yellow and green lines in fig. 2). Finally, in fig. 3, we show the effect of dimension on the energy levels. When N increase the energy increase too, but it has more effect on lower states (compare yellow and green lines in fig. 2) and it can be seen that the energy eigenvalues decrease from $N = 1$ to 3 and next increase.

To find corresponding wave functions, referring to table 1 and Eq. (11), we get the radial wave functions as

$$R_{nl}(s) = N_{nl}s^{\sqrt{\xi_3}}(1+s)^{2-\sqrt{\xi_1+\xi_2+\xi_3+4}}P_n^{(2\sqrt{\xi_3},-2\sqrt{\xi_1+\xi_2+\xi_3+4})}(1+2s), \tag{22}$$

where N_{nl} is normalization constant.

4. Conclusions

In this work, by using an improved approximation scheme to the centrifugal barrier term, we obtained approximate solutions of the generalized Morse or Deng-Fan potential by using the generalized parametric NU method. The bound state eigenvalues and corresponding wave functions are given in their closed forms and some numerical are given in table 2 and figures 1-3.

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Table 1. The specific values for the parametric constants necessary for the energy eigenvalues and eigenfunctions

constant	Analytic value
α_4	0
α_5	2
α_6	ξ_1+4
α_7	$-\xi_2$
α_8	ξ_3
α_9	$\xi_1+\xi_2+\xi_3+4$
α_{10}	$1+2\sqrt{\xi_3}$
α_{11}	$-2+2(\sqrt{\xi_1+\xi_2+\xi_3+4}-\sqrt{\xi_3})$
α_{12}	$\sqrt{\xi_3}$
α_{13}	$2-2(\sqrt{\xi_1+\xi_2+\xi_3+4}-\sqrt{\xi_3})$

Table 2: The bound state energy eigenvalues in unit of fm^{-1} of the Deng-Fan potential for several values of N , a , n and l with $r_e=0.4$.

N	a	$E_{0,0}$	$E_{1,0}$	$E_{2,0}$	$E_{2,1}$	$E_{3,0}$	$E_{3,1}$	$E_{3,2}$
1	0.05	24.27018562	25.30058361	26.10047156	26.10047156	26.73987630	26.73987630	26.78826883
	0.1	24.28339946	25.34681569	26.17301149	26.17301149	26.83396562	26.83396562	26.88369749
	0.2	24.31021499	25.43910469	26.31675842	26.31675842	27.01918275	27.01918275	27.07185245
2	0.05	24.25699802	25.29072173	26.09279898	26.12332466	26.73373839	26.75817046	26.82960600
	0.1	24.26989522	25.33670832	26.16513868	26.19646383	26.82765954	26.85276331	26.92619758
	0.2	24.29602915	25.42846531	26.30844894	26.34151775	27.01250785	27.03908477	27.11690447
3	0.05	24.27018562	25.30058361	26.10047156	26.16087452	26.73987630	26.78826883	26.88143276
	0.1	24.28339946	25.34681569	26.17301149	26.23500758	26.83396562	26.88369749	26.97950697
	0.2	24.31021499	25.43910469	26.31675842	26.38222961	27.01918275	27.07185245	27.17346896
4	0.05	24.30937431	25.32993043	26.12332466	26.21234736	26.75817046	26.82960600	26.94285303
	0.1	24.32353359	25.37689666	26.19646383	26.28786164	26.85276331	26.92619758	27.04271985
	0.2	24.35238431	25.47077674	26.34151775	26.43809756	27.03908477	27.11690447	27.24062020
5	0.05	24.37347330	25.37806263	26.16087452	26.27672408	26.78826883	26.88143276	27.01286457
	0.1	24.38919356	25.42624470	26.23500758	26.35399651	26.88369749	26.97950697	27.11482195
	0.2	24.42140475	25.52276011	26.38222961	26.50807054	27.07185245	27.17346896	27.31731938
6	0.05	24.46076434	25.44386795	26.21234736	26.35279512	26.82960600	26.94285303	27.09040022
	0.1	24.47863975	25.49373600	26.28786164	26.43218929	26.92619758	27.04271985	27.19473183
	0.2	24.51549117	25.59390660	26.43809756	26.59089791	27.11690447	27.24062020	27.40245606
7	0.05	24.56903356	25.52589403	26.27672408	26.43922016	26.88143276	27.01286457	27.17436659
	0.1	24.58962977	25.57790220	26.35399651	26.52108327	26.97950697	27.11482195	27.28133972
	0.2	24.63234080	25.68271431	26.50807054	26.68518938	27.17346896	27.31731938	27.49488737
8	0.05	24.69572592	25.62243602	26.35279512	26.53458695	26.94285303	27.09040022	27.26367812
	0.1	24.71957410	25.67701834	26.43218929	26.61924714	27.04271985	27.19473183	27.37354190
	0.2	24.76929159	25.78741623	26.59089791	26.78947459	27.24062020	27.40245606	27.59347296
9	0.05	24.83810163	25.73162924	26.43922016	26.63746521	27.01286457	27.17436659	27.35728534
	0.1	24.86569389	25.78919583	26.52108327	26.72522911	27.11482195	27.28133972	27.47026928
	0.2	24.92348310	25.90607423	26.68518938	26.90225799	27.31731938	27.49488737	27.69710422
10	0.05	24.99337834	25.85153773	26.53458695	26.74645252	27.09040022	27.26367812	27.45419662
	0.1	25.02516446	25.91247154	26.61924714	26.83760327	27.19473183	27.37354190	27.57050952
	0.2	25.09200290	26.03666928	26.78947459	27.02206603	27.40245606	27.59347296	27.80472724

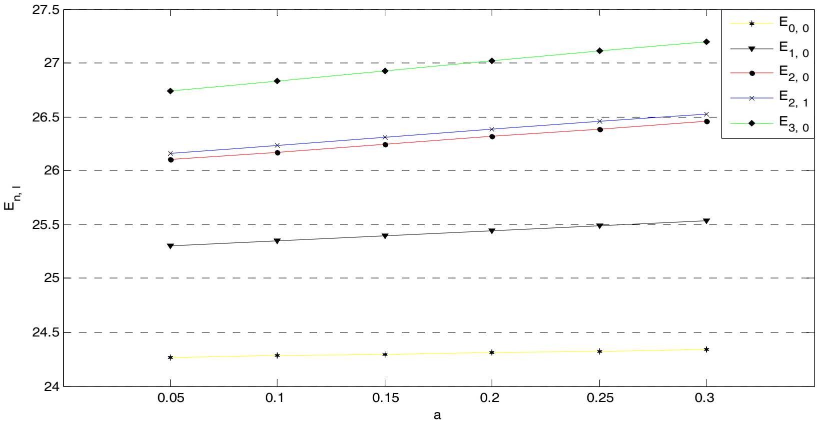

Fig. 1: Energy behavior versus a for $N=3$ and various n,l s.

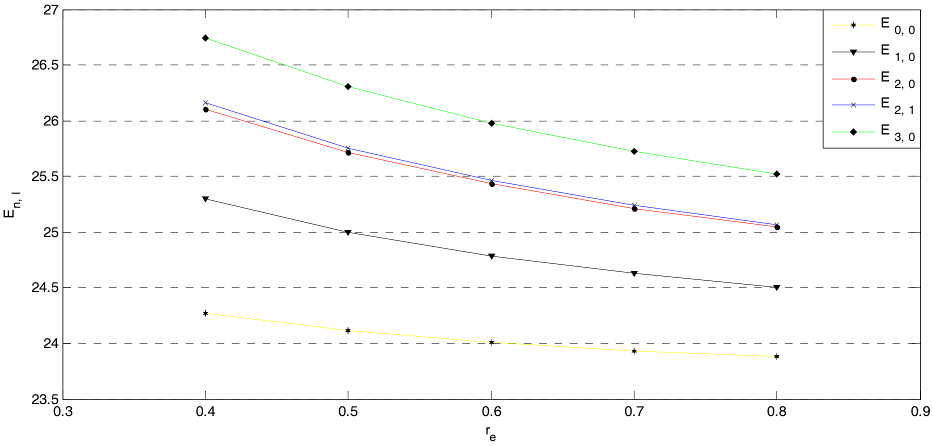

Fig. 2: Energy behavior versus r_e for $N=3$ and various n,l s.

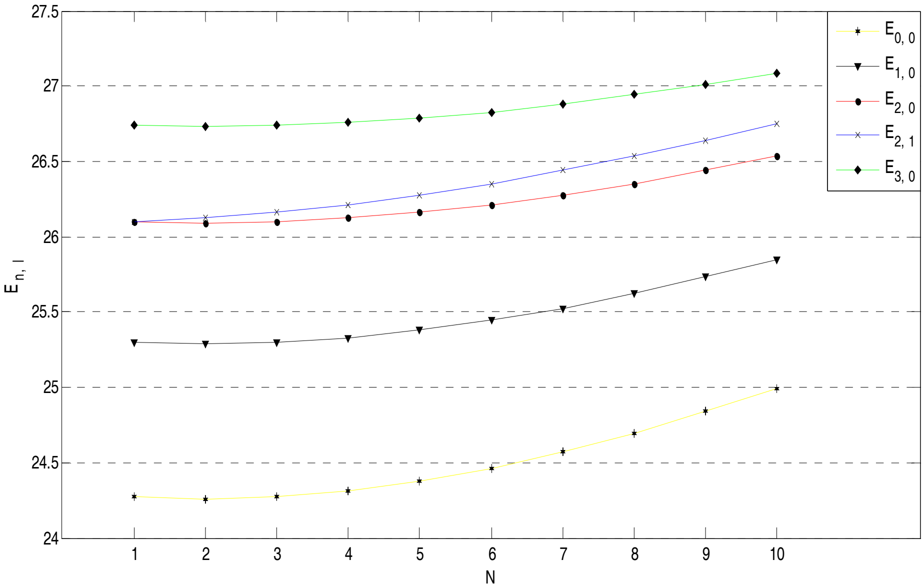

Fig. 3: Energy behavior versus N for various n, l s.